Perturbation Expansion of the Partition Sum for any Temperature

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Abstract

Based on the special properties of Liouville eigenoperators a perturbation theory for the partition sum is given. It is applicable for any temperature and includes the case of degenerate Hamiltonians. To demonstrate the realibility of the method, the second order correction to the atomic limit grand canonical potential of the Hubbard model is calculated and compared to results known from the literature.

1 Introduction

From the early beginning of statistical thermodynamics there was no doubt that the partition sum is the central quantity for describing the equilibrium quantities in physics. In spite of its central role there is no easy to handle perturbation theory for arbitrary temperature up to now. Of course, from the first days of quantum mechanics there were attempts in this direction. They all suffer from the non-commutativity of the perturbation with the unperturbed Hamiltonian, which makes it necessary to introduce an imaginary time via the Feynmann time ordering trick to split the exponential contained in the partition sum, resulting in various graph schemes for perturbation series or two time Green functions. Of course, perturbation theories are widely employed in all fields of contemporary physics and, therefore, it is hopeless to review all the developments, so I restrict to a brief review of the state of art in the context of the Hubbard model [1, 2], a basic model in condensed matter physics due to its relevance for strong electron correlation phenomena like itinerant magnetism or, for meanwhile ten years, high T_C superconductivity [3]. In 1980 Kubo [4] published a high temperature expansion, and the nowadays developed cumulant expansions [5, 6] and in future the incremental method [7] seems to have the potential for a break through in the direction towards arbitrary temperatures. Nevertheless, at the moment the latter theories are mainly elaborated for the ground state properties, whereas the finite temperature business was left aside. Another way, which was shown to be equivalent to the cumulant technique [9] at least for the ground state, is the coupled cluster expansion [10]. An extension to finite temperature was given in [15]. In [8] an algebraic approach to operator perturbation theory was presented for zero temperature, nevertheless an extension to finite temperatures seems to be possible also in this line. The series expansion for the thermodynamical potential can

be generated from series expansion of the one particle green function, what of course also introduces (imaginary) time variables. In the following we will develope a series expansion avoiding this difficulty.

2 The perturbation series for the partition sum

We assume, that the system under consideration is described by a Hamiltonian $\boldsymbol{H}$, which can be splitted into two parts, i.e.

$$\boldsymbol{H} = \boldsymbol{H}_0 + \boldsymbol{H}_1\,, \tag{1}$$

The partitition sum is

$$Z \;=\; Sp\left\{e^{-\beta(\boldsymbol{H}_0 + \boldsymbol{H}_1)}\right\} \tag{2}$$

This can be rewritten in the following form

$$Z \;=\; Sp\left\{e^{-\beta\boldsymbol{H}_0}\boldsymbol{S}(\beta)\right\} \tag{3}$$

with

$$\boldsymbol{S}(\beta) \;=\; e^{\beta\boldsymbol{H}_0}e^{-\beta\boldsymbol{H}} \tag{4}$$

The perturbation expansion for the operator $S(\beta)$ given in various textbooks on quantum statistics is

$$\boldsymbol{S}(\beta) = \sum_{n=0}^{\infty}(-1)^n \int_0^\beta d\beta_1 \int_0^{\beta_1} d\beta_2 \cdots \int_0^{\beta_{n-1}} d\beta_n \boldsymbol{H}_1(\beta_1)\boldsymbol{H}_1(\beta_2)\cdots\boldsymbol{H}_1(\beta_n) \tag{5}$$

with $\boldsymbol{H}_1(\tau)$ being

$$\boldsymbol{H}_1(\tau) \;=\; e^{\tau\boldsymbol{H}_0}\boldsymbol{H}_1 e^{-\tau\boldsymbol{H}_0} \tag{6}$$

It is this (imaginary) time dependence and the multiple time integrals which makes the calculation of the perturbation series involved. In the following we show that one can get rid of this problem. For that, we consider both parts of the Hamiltonian as elements of the same operator space, and, therefore, $\boldsymbol{H}_1$ can be expressed in terms of eigenoperators of the Liouvillian belonging to $\boldsymbol{H}_0$. The Liouvillian of a Hamiltonian is defined as

$$\boldsymbol{L}\boldsymbol{A} \;=\; [\boldsymbol{H}, \boldsymbol{A}] \tag{7}$$

and an eigenoperator $\boldsymbol{A}$ fullfills the eigenvalue equation

$$\boldsymbol{L}\boldsymbol{A} \;=\; \lambda_A\boldsymbol{A}\,. \tag{8}$$

The product of two eigenoperators $\boldsymbol{A}$ and $\boldsymbol{B}$ is also an eigenoperator, with

$$\boldsymbol{L}(\boldsymbol{A}\boldsymbol{B}) \;=\; (\boldsymbol{L}\boldsymbol{A})\boldsymbol{B} + \boldsymbol{A}(\boldsymbol{L}\boldsymbol{B}) = \lambda_A\boldsymbol{A}\boldsymbol{B} + \boldsymbol{A}\lambda_B\boldsymbol{B} = (\lambda_A + \lambda_B)(\boldsymbol{A}\boldsymbol{B}) \tag{9}$$

Next, we expand the $\boldsymbol{S}$ from eq (4) into a Taylor series

$$\boldsymbol{S}(\beta) \; = \; \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \left[\frac{\partial^n}{\partial \beta^n} \boldsymbol{S}(\beta) \right]_{\beta=0} \tag{10}$$

For the first derivative of $\boldsymbol{S}$ we find

$$\frac{\partial}{\partial \beta} \boldsymbol{S}(\beta) \; = \; \boldsymbol{a}_{11}(\beta) \boldsymbol{S}(\beta) \tag{11}$$

with

$$\boldsymbol{a}_{11}(\beta) \; = \; e^{\beta \boldsymbol{H}_0} \boldsymbol{a}_{11} e^{-\beta \boldsymbol{H}_0} = -e^{\beta \boldsymbol{H}_0} \boldsymbol{H}_1 e^{-\beta \boldsymbol{H}_0} \tag{12}$$

The operator $\boldsymbol{a}_{11}$ is first order in the perturbation. The second derivative is

$$\begin{aligned}
\frac{\partial^2}{\partial \beta^2} \boldsymbol{S}(\beta) \; &= \; \left(\frac{\partial}{\partial \beta} \boldsymbol{a}_{11}(\beta) + \boldsymbol{a}_{11}(\beta) \boldsymbol{a}_{11}(\beta) \right) \boldsymbol{S}(\beta) \\
&= \; \left(\boldsymbol{a}_{21}(\beta) + \boldsymbol{a}_{22}(\beta) \right) \boldsymbol{S}(\beta)
\end{aligned} \tag{13}$$

Since the derivation of an $\boldsymbol{a}$-operator with respect to β does not increase the order of the perturbation $\boldsymbol{a}_{21}(\beta)$ remains first order whereas $\boldsymbol{a}_{22}(\beta) = \boldsymbol{a}_{11}^2(\beta)$ is second order. The next derivative is

$$\frac{\partial^3}{\partial \beta^3} \boldsymbol{S}(\beta) \; = \; \left(\frac{\partial}{\partial \beta} \boldsymbol{a}_{21}(\beta) + \frac{\partial}{\partial \beta} \boldsymbol{a}_{22}(\beta) + (\boldsymbol{a}_{21}(\beta) + \boldsymbol{a}_{22}(\beta)) \boldsymbol{a}_{11}(\beta) \right) \boldsymbol{S}(\beta) \tag{14}$$

Collecting together terms of the same order in the perturbation yields

$$\frac{\partial^3}{\partial \beta^3} \boldsymbol{S}(\beta) \; = \; \left(\boldsymbol{a}_{31}(\beta) + \boldsymbol{a}_{32}(\beta) + \boldsymbol{a}_{33}(\beta) \right) \boldsymbol{S}(\beta) \tag{15}$$

Proceeding in this way we can sort the summands contributing to the expansion of $\boldsymbol{S}$ in a table. Since the derivatives have to be taken at infinite temperature (i.e. at $\beta = 0$) we have $\boldsymbol{S}_0 = 1$. Furthermore, the derivative of an $\boldsymbol{a}_{nm}$ with respect to β taken at $\beta = 0$ is nothing but applying the Liouvillian to that operator. In table 1 the column index gives the order in the perturbation whereas the row index gives the order in β. Thus by resorting the sum one finds

$$\boldsymbol{S}(\beta) \; = \; 1 + \boldsymbol{S}_1(\beta) + \boldsymbol{S}_2(\beta) + \boldsymbol{S}_3(\beta) + \cdots \tag{16}$$

with

$$\boldsymbol{S}_m(\beta) \; = \; \sum_{n=m}^{\infty} \frac{\beta^n}{n!} \boldsymbol{a}_{nm} \tag{17}$$

It is easy to show that for the operators $\boldsymbol{a}_{mn}$ the following recursion relations hold

$$\boldsymbol{a}_{mm} \; = \; \boldsymbol{a}_{11}^m \tag{18}$$

$$\boldsymbol{a}_{n1} \; = \; \boldsymbol{L}_0^{n-1} \boldsymbol{a}_{11} \tag{19}$$

$$\boldsymbol{a}_{nm} \; = \; \boldsymbol{L}_0 \boldsymbol{a}_{n-1\,m} + \boldsymbol{a}_{n-1\,m-1} \boldsymbol{a}_{11} \tag{20}$$

	1.	2.	3.	4.
$\frac{\beta}{1!}$	$\boldsymbol{a}_{11}$			
	$\downarrow \boldsymbol{L}_0 \quad \searrow \times \boldsymbol{a}_{11}$			
$\frac{\beta^2}{2!}$	$\boldsymbol{a}_{21}$	$\boldsymbol{a}_{22}$		
	$\downarrow \boldsymbol{L}_0 \quad \searrow \times \boldsymbol{a}_{11}$	$\downarrow \boldsymbol{L}_0 \quad \searrow \times \boldsymbol{a}_{11}$		
$\frac{\beta^3}{3!}$	$\boldsymbol{a}_{31}$	$\boldsymbol{a}_{32}$	$\boldsymbol{a}_{33}$	
	$\downarrow \boldsymbol{L}_0 \quad \searrow \times \boldsymbol{a}_{11}$	$\downarrow \boldsymbol{L}_0 \quad \searrow \times \boldsymbol{a}_{11}$	$\downarrow \boldsymbol{L}_0 \quad \searrow \times \boldsymbol{a}_{11}$	
$\frac{\beta^4}{4!}$	$\boldsymbol{a}_{41}$	$\boldsymbol{a}_{42}$	$\boldsymbol{a}_{43}$	$\boldsymbol{a}_{44}$

Table 1: Operators $\boldsymbol{a}_{nm}$ of the same order in the perturbation are depicted in the columns. The rows give the operators contributing to the same power of the temperature. The arrows symbolize the recursive connection between the operators. A vertical arrow stands for application of $\boldsymbol{L}_0$ and a slanted arrow for post-multiplying with $\boldsymbol{a}_{11}$.

By help of the above equations (20) the following formula results

$$\boldsymbol{a}_{nm} = \boldsymbol{L}_0^{n-m}\boldsymbol{a}_{mm} + \sum_{k=0}^{n-1-m} \boldsymbol{L}_0^k(\boldsymbol{a}_{n-1-k\,m-1}\boldsymbol{a}_{11}) \tag{21}$$

The recursion relations allow to find closed formula for the m-th order contribution to the partition sum. We will show this explicit for the second order contribution and the third order contribution respectively. Summing the second and the third column in table 1 respectively yields for the operators $\boldsymbol{S}_2$ and $\boldsymbol{S}_3$

$$\boldsymbol{S}_2 = \sum_{n=2}^{\infty} \frac{\beta^n}{n!}\boldsymbol{a}_{n2} \quad ; \quad \boldsymbol{S}_3 = \sum_{n=3}^{\infty} \frac{\beta^n}{n!}\boldsymbol{a}_{n3} \tag{22}$$

Iterating eq (21) one gets for the operators $\boldsymbol{a}_{n2}$

$$\boldsymbol{a}_{n2} = \delta_{n,2}\boldsymbol{a}_{22} + \delta_{n>2}\left\{ \boldsymbol{L}_0^{n-2}\boldsymbol{a}_{22} + \sum_{k=0}^{n-3} \boldsymbol{L}_0^k(\boldsymbol{a}_{n-1-k\,1}\boldsymbol{a}_{11}) \right\}$$

$$= \delta_{n,2}\boldsymbol{a}_{22} + \delta_{n>2}\left\{ \boldsymbol{L}_0^{n-2}\boldsymbol{a}_{22} + \sum_{k=0}^{n-3} \boldsymbol{L}_0^k\left[(\boldsymbol{L}_0^{n-1-k}\boldsymbol{a}_{11})\boldsymbol{a}_{11}) \right] \right\} \tag{23}$$

Here the shortcut $\delta_{n>m}$ says that n has to be greater than m. For the third order results

$$\boldsymbol{a}_{n3} = \delta_{n,3}\,\boldsymbol{a}_{33} + \delta_{n>3}\,\boldsymbol{L}_0^{n-3}\boldsymbol{a}_{33} +$$

$$+\delta_{n>3}\left\{\sum_{k=0}^{n-4}\boldsymbol{L}_0^k\left(\boldsymbol{L}_0^{n-3-k}\boldsymbol{a}_{22}+\sum_{l=0}^{n-4-k}\boldsymbol{L}_0^l\left[(\boldsymbol{L}_0^{n-3-k-l}\boldsymbol{a}_{11})\boldsymbol{a}_{11}\right]\boldsymbol{a}_{11}\right)\right\} \tag{24}$$

One finds with eqs (3,17) for the m-th order contribution to the partition sum

$$Z_m/Z_0 \;=\; Sp\left\{e^{-\beta\boldsymbol{H}_0}\sum_{n=m}^{\infty}\frac{\beta^n}{n!}\boldsymbol{a}_{nm}\right\}=\sum_{n=m}^{\infty}\frac{\beta^n}{n!}\langle\boldsymbol{a}_{nm}\rangle \tag{25}$$

what can be rewritten by help of eq (21)

$$Z_m/Z_0 \;=\; \sum_{n=m}^{\infty}\frac{\beta^n}{n!}\left\{\langle\boldsymbol{L}_0^{n-m}\boldsymbol{a}_{mm}\rangle+\delta_{n>m}\sum_{k=0}^{n-1-m}\langle\boldsymbol{L}_0^k(\boldsymbol{a}_{n-1-k,m-1}\boldsymbol{a}_{11})\rangle\right\} \tag{26}$$

Since for every operator $\boldsymbol{A}$ holds

$$\langle\boldsymbol{L}_0^{n-m}\boldsymbol{A}\rangle \;=\; \delta_{nm}\langle\boldsymbol{A}\rangle \tag{27}$$

we find

$$Z_m/Z_0 \;=\; \frac{\beta^m}{m!}\langle\boldsymbol{a}_{mm}\rangle+\sum_{n=m+1}^{\infty}\frac{\beta^n}{n!}\langle\boldsymbol{a}_{n-1,m-1}\boldsymbol{a}_{11}\rangle \tag{28}$$

the next recursion step yields

$$Z_m/Z_0 \;=\; \frac{\beta^m}{m!}\langle\boldsymbol{a}_{mm}\rangle+\sum_{n=m+1}^{\infty}\frac{\beta^n}{n!}\langle(\boldsymbol{L}_0^{n-m}\boldsymbol{a}_{m-1,m-1})\boldsymbol{a}_{11}\rangle$$
$$+\sum_{n=m+1}^{\infty}\frac{\beta^n}{n!}\sum_{k=0}^{n-1-m}\langle\left(\boldsymbol{L}_0^k(\boldsymbol{a}_{n-2-k,m-2}\boldsymbol{a}_{11})\right)\boldsymbol{a}_{11}\rangle \tag{29}$$

The recursion ends when the operators are reduced to products of $\boldsymbol{a}_{11}$. Thus we get for the second order from eq (28)

$$Z_2/Z_0 \;=\; \frac{\beta^2}{2!}\langle\boldsymbol{a}_{22}\rangle+\sum_{n=3}^{\infty}\frac{\beta^n}{n!}\langle\boldsymbol{a}_{n-11}\boldsymbol{a}_{11}\rangle$$
$$=\; \frac{\beta^2}{2!}\langle\boldsymbol{a}_{11}^2\rangle+\sum_{n=3}^{\infty}\frac{\beta^n}{n!}\langle(\boldsymbol{L}_0^{n-2}\boldsymbol{a}_{11})\boldsymbol{a}_{11}\rangle \tag{30}$$

and for the third order

$$Z_3/Z_0 \;=\; \frac{\beta^3}{3!}\langle\boldsymbol{a}_{33}\rangle+\sum_{n=4}^{\infty}\frac{\beta^n}{n!}\langle\left(\boldsymbol{L}_0^{n-3}\boldsymbol{a}_{22}\right)\boldsymbol{a}_{11}\rangle+\sum_{n=4}^{\infty}\frac{\beta^n}{n!}\sum_{l=0}^{n-4}\langle\left(\boldsymbol{L}_0\left(\boldsymbol{L}_0^{n-3-l}\boldsymbol{a}_{11}\right)\boldsymbol{a}_{11}\right)\boldsymbol{a}_{11}\rangle$$
$$=\; \frac{\beta^3}{3!}\langle\boldsymbol{a}_{11}^3\rangle+\sum_{n=4}^{\infty}\frac{\beta^n}{n!}\langle\left(\boldsymbol{L}_0^{n-3}\boldsymbol{a}_{11}^2\right)\boldsymbol{a}_{11}\rangle+\sum_{n=4}^{\infty}\frac{\beta^n}{n!}\sum_{l=0}^{n-4}\langle\left(\boldsymbol{L}_0\left(\boldsymbol{L}_0^{n-3-l}\boldsymbol{a}_{11}\right)\boldsymbol{a}_{11}\right)\boldsymbol{a}_{11}\rangle \tag{31}$$

Next, the perturbation $\boldsymbol{H}_1$ is decomposed into eigenoperators of $\boldsymbol{L}_0$. For that we use the natural basis of the Liouville space formed by the dyades constructed from the eigenstates of $\boldsymbol{H}_0$. In this representation $\boldsymbol{H}_0$ is diagonal and $\boldsymbol{H}_1$ is chosen purely offdiagonal, what is

always possible. In case that $\boldsymbol{H}_1$ contains components which are diagonal they are added to $\boldsymbol{H}_0$.

$$\boldsymbol{H}_0 = \sum_\nu \varepsilon_\nu |\nu\rangle\langle\nu| \qquad \text{with} \qquad \boldsymbol{H}_0|\nu\rangle = \varepsilon_\nu|\nu\rangle . \tag{32}$$

and

$$\boldsymbol{H}_1 = \sum_\mu \sum_\nu V_{\mu\nu}|\mu\rangle\langle\nu| \tag{33}$$

The basis operators $|\mu\rangle\langle\nu|$ are eigenoperators of the Liouvillian $\boldsymbol{L}_0$ following

$$\boldsymbol{L}_0|\mu\rangle\langle\nu| = \lambda_{\mu\nu}|\mu\rangle\langle\nu| \qquad \text{with} \qquad \lambda_{\mu\nu} = \varepsilon_\mu - \varepsilon_\nu \tag{34}$$

For the operator $\boldsymbol{a}_{11}$ we get

$$\boldsymbol{a}_{11} = \sum_\mu \sum_\nu A_{\mu\nu}|\mu\rangle\langle\nu| \qquad \text{with} \qquad A_{\mu\nu} = -V_{\mu\nu} \tag{35}$$

By insertion of the above expression into eqs (30,31) and using the linearity of the Liouvillian the result for the second order contribution to the partition sum is

$$Z_2 = \sum_\mu \sum_\nu e^{-\beta\varepsilon_\mu} V_{\mu\nu} V_{\nu\mu} f_2(\lambda_1) \tag{36}$$

with

$$f_2(\lambda_1) = \frac{\beta^2}{2!} + \frac{E_2(\lambda_1)}{\lambda_1^2} \tag{37}$$

and the third order contribution reads as

$$Z_3 = -\sum_\mu \sum_\nu \sum_\alpha e^{-\beta\varepsilon_\mu} V_{\mu\nu} V_{\nu\alpha} V_{\alpha\mu} f_3(\lambda_1, \lambda_2) \tag{38}$$

with

$$f_3(\lambda_1, \lambda_2) = \frac{\beta^3}{3!} + \frac{1}{\lambda_2 - \lambda_1}\frac{E_3(\lambda_1)}{\lambda_1^2} + \frac{1}{\lambda_1 - \lambda_2}\frac{E_3(\lambda_2)}{\lambda_2^2} \tag{39}$$

Here we introduced the functions $E_m(\lambda)$, which are determined according to

$$E_m(\lambda) = e^{\beta\lambda} - \sum_{n=0}^{m} \frac{(\beta\lambda)^n}{n!} \tag{40}$$

Furthermore we abbreviated

$$\lambda_1 = \lambda_{\mu\mu'} \tag{41}$$
$$\lambda_2 = \lambda_{\mu\mu'} + \lambda_{\nu\nu'} \tag{42}$$

In the same way we proceeded to higher orders in the perturbation. We calculated the coefficients to the eighth order terms, what one finds for the mth-order contribution to the partition sum is

$$Z_m = (-1)^m \sum_{\mu_1} \cdots \sum_{\mu_m} e^{-\beta \varepsilon_{\mu_1}} V_{\mu_1 \mu_2} V_{\mu_2 \mu_3} \cdots V_{\mu_{m-1} \mu_m} V_{\mu_m \mu_1} f_m(\lambda_1, \ldots, \lambda_{m-1}) \tag{43}$$

with

$$f_m(\lambda_1, \ldots, \lambda_{m-1}) = \frac{\beta^m}{m!} + \sum_{i=1}^{m-1} \frac{\lambda_i^{m-2}}{\prod_{j \neq i}(\lambda_j - \lambda_i)} \frac{E_m(\lambda_i)}{\lambda_i^m} \tag{44}$$

and

$$\lambda_k = \lambda_{\mu_1 \mu_2} + \lambda_{\mu_2 \mu_3} + \cdots + \lambda_{\mu_k \mu_{k+1}} = \varepsilon_{\mu_1} - \varepsilon_{\mu_k} \tag{45}$$

We want to emphasize, that the functions $f_m(\lambda_1, \cdots, \lambda_{m-1})$ remain finite for any number of vanishing λ_i, and, therefore, the case that the unperturbed Hamiltonian has a degenerated spectrum is included. Furthermore, it remains finite for all values of β . This becomes immediately clear, if one looks at the structure of the operators $\boldsymbol{a}_{nm}$, which do not contain any denominators, e.g. look at $\boldsymbol{a}_{n2}$ and $\boldsymbol{a}_{n3}$ as given in eqs (23) and (24) respectively. Eq (43) provides a compact form for the perturbation series of the partition sum which can be tested easily for simple systems. As will be shown in the following the functions $f_m(\lambda_1, \cdots, \lambda_{m-1})$ are nothing but the result of the m-1 integrations necessary in standard perturbation theory. Thus we did this integrals to infinite order. Starting from eq (5) we can insert the perturbation in the form given in eq (33), what yields

$$Z(\beta) = \sum_{m=0}^{\infty} (-1)^m \sum_{\nu_1} \sum_{\nu_2} \cdots \sum_{\nu_m} e^{-\beta \varepsilon_{\nu_1}} V_{\nu_1, \nu_2} V_{\nu_2, \nu_3} \cdots V_{\nu_m, \nu_1} \times \tag{46}$$

$$\times \int_0^{\beta} d\beta_1 \int_0^{\beta_1} d\beta_2 \cdots \int_0^{\beta_{m-1}} d\beta_m e^{\beta_1(\varepsilon_{\nu_1} - \varepsilon_{\nu_2})} e^{\beta_2(\varepsilon_{\nu_2} - \varepsilon_{\nu_3})} \ldots e^{\beta_m(\varepsilon_{\nu_m} - \varepsilon_{\nu_1})}$$

due to the eigenvalue equation of the unperturbed Hamiltonian for the partition sum. It is obvious that the result of the m integrations have to be the same as the functions introduced in eq (44). Taking into account the definitions of the λ_i one finds

$$\varepsilon_{\nu_1} - \varepsilon_{\nu_2} = \lambda_1 \tag{47}$$
$$\varepsilon_{\nu_i} - \varepsilon_{\nu_{i+1}} = -\lambda_{i-1} + \lambda_i \quad \text{with} \quad 1 < i < m \tag{48}$$

and, therefore,

$$f_m(\lambda_1, \ldots, \lambda_{m-1}) = \int_0^{\beta} d\beta_1 \int_0^{\beta_1} d\beta_2 \cdots \int_0^{\beta_{m-1}} d\beta_m e^{\beta_1 \lambda_1} e^{\beta_2(-\lambda_1 + \lambda_2)} \ldots e^{\beta_m(-\lambda_{m-1})} \tag{49}$$

These integrals were calculated by help of symbolic computer programs. Up to order five (2^5 terms), it was possible to bring the results symbolically to the forms given in eq. (44)

by help of the tools, the symbolic computer languages provide. For the sixth, seventh, and eighth order term we proved it by numerical calculation, for arbitrary sets of λ's, and found reasonable coincidence within the numerical error. A different way to do the integrals is by help of Laplace's transformation [20]. This results in a form of f_m which seems at the first glance different. Nevertheless it can be shown to be equivalent to eq (44). The calculation is given in the appendix D. For comparison with the literature, where results are given for the series expansion of the grand potential, we have to express the perturbation series for the grand potential F via the perturbation series of the partition sum. One finds easily

$$
\begin{aligned}
\beta F &= \beta F_0 + \beta F_2 + \beta F_3 + \beta F_4... \\
&= -\log Z_0 - \frac{Z_2}{Z_0} - \frac{Z_3}{Z_0} - \left(\frac{Z_4}{Z_0} - \frac{Z_2^2}{Z_0^2}\right) + ...
\end{aligned}
\tag{50}
$$

This expression may be compared to the usual perturbation theory for the grand potential [21]

$$
\beta F = \beta F_0 - \sum_{n=2}^{\infty} (-1)^n \int_0^\beta d\beta_1 \int_0^{\beta_1} d\beta_2 \cdots \int_0^{\beta_{n-1}} d\beta_n \langle \boldsymbol{H}_1(\beta_1)\boldsymbol{H}_1(\beta_2)\cdots\boldsymbol{H}_1(\beta_n)\rangle^c
\tag{51}
$$

here $\langle\ldots\rangle^c$ indicates that cumulants [5] have to be calculated. Due to the linearity of cumulants we can separate the τ-integrations what yields together with eq (49)

$$
\begin{aligned}
\beta F &= \beta F_0 - \sum_{n=2}^{\infty} (-1)^n \sum_{\mu_1} \cdots \sum_{\mu_n} e^{-\beta\varepsilon_{\mu_1}} f_n(\lambda_1,\ldots,\lambda_{n-1}) \times \\
&\quad \times \langle V_{\mu_1\mu_2} V_{\mu_2\mu_3} \cdots V_{\mu_{n-1}\mu_n} V_{\mu_n\mu_1}\rangle^c
\end{aligned}
\tag{52}
$$

Thus it is sufficient to calculate cumulants, i.e. the linked graphs.

3 Calculating the expectation values

What remains to calculate is the expectation value of eigenoperator products, being of the form

$$
\langle \boldsymbol{AB}\rangle = \frac{1}{Z_0} Sp\left\{e^{-\beta\boldsymbol{H}_0}\boldsymbol{AB}\right\}
\tag{53}
$$

Here $\boldsymbol{A}$ is an arbitrary eigenoperator of $\boldsymbol{L}_0$ with eigenvalue λ_A and $\boldsymbol{B}$ any other operator, $\langle\cdots\rangle$ is again the expectation value with respect to the unperturbed Hamiltonian . Since cyclic permutations under a trace do not alter the expectation value we find

$$
\begin{aligned}
Sp\left\{e^{-\beta\boldsymbol{H}_0}\boldsymbol{AB}\right\} &= Sp\left\{\left(e^{-\beta\boldsymbol{L}_0}\boldsymbol{A}\right)e^{-\beta\boldsymbol{H}_0}\boldsymbol{B}\right\} = e^{-\beta\lambda_A} Sp\left\{e^{-\beta\boldsymbol{H}_0}\boldsymbol{BA}\right\} \\
&= e^{-\beta\lambda_A} Sp\left\{e^{-\beta\boldsymbol{H}_0}[\boldsymbol{B},\boldsymbol{A}]_+\right\} - e^{-\beta\lambda_A} Sp\left\{e^{-\beta\boldsymbol{H}_0}\boldsymbol{AB}\right\}
\end{aligned}
\tag{54}
$$

Solving for $\langle \boldsymbol{AB} \rangle$ yields

$$\langle \boldsymbol{AB} \rangle = \frac{1}{e^{\beta \lambda_A} + 1} \langle [\boldsymbol{A}, \boldsymbol{B}]_+ \rangle \tag{55}$$

If $\boldsymbol{B}$ is an eigenoperator instead of $\boldsymbol{A}$ one finds in the same way

$$\langle \boldsymbol{AB} \rangle = \frac{1}{e^{-\beta \lambda_B} + 1} \langle [\boldsymbol{A}, \boldsymbol{B}]_+ \rangle \tag{56}$$

Of course one can get these results also via the standard Green function technique which becomes extremly simple for eigenoperators. This is shown in appendix A. If both $\boldsymbol{A}$ and $\boldsymbol{B}$ are eigenoperators, than one has

$$
\begin{aligned}
Sp\left\{e^{-\beta \boldsymbol{H}_0} \boldsymbol{AB}\right\} &= Sp\left\{e^{-\beta \boldsymbol{H}_0} \boldsymbol{AB} e^{\beta \boldsymbol{H}_0} e^{-\beta \boldsymbol{H}_0}\right\} \\
&= Sp\left\{\left(e^{-\beta \boldsymbol{L}_0} \boldsymbol{AB}\right) e^{-\beta \boldsymbol{H}_0}\right\} = e^{-\beta(\lambda_A + \lambda_B)} Sp\left\{e^{-\beta \boldsymbol{H}_0} \boldsymbol{AB}\right\}
\end{aligned} \tag{57}
$$

It follows that either the expectation values $\langle \boldsymbol{AB} \rangle$ and $\langle \boldsymbol{BA} \rangle$ vanish or the equation

$$\lambda_B = -\lambda_A \qquad \text{for } \boldsymbol{A}, \boldsymbol{B} \text{ eigenoperators of } \boldsymbol{L}_0 \tag{58}$$

holds. In some models, e.g. within the Hubbard model, the operators $\boldsymbol{A}$ and $\boldsymbol{B}$ may be both fermionic and bosonic. If both operators are fermionic, than the anticommutator is suitable, since the number of operators will be reduced. In case that at least one of the operators $\boldsymbol{A}$ or $\boldsymbol{B}$ is bosonic, than its more convenient to work with the commutator. The related formula can be derived easily from eq (55) to be

$$\langle \boldsymbol{AB} \rangle = \frac{1}{1 - e^{\beta \lambda_A}} \langle [\boldsymbol{A}, \boldsymbol{B}] \rangle \tag{59}$$

Introducing a "parity function" $P(\boldsymbol{A}|\boldsymbol{B})$ being an odd integer if both operators are fermionic and even else one can unite eqs (55,59) in the following way

$$\langle \boldsymbol{AB} \rangle = \frac{1}{1 - (-1)^{P(A|B)} e^{\beta \lambda_A}} \langle \boldsymbol{AB} - (-1)^{P(A|B)} \boldsymbol{BA} \rangle \tag{60}$$

In the above form the number of operators will be always reduced. It is of some interest to discuss the case when the denominator in eq (59) vanishes. This may happen if the temperature goes to infinity. Since there is no reason that the expectation value $\langle \boldsymbol{AB} \rangle$ becomes infinite, we have to conclude, that the commutator becomes zero, what represents the classical limit. More interesting is the case that the eigenvalue λ_A is zero. But this implies the following statement: If the operator $\boldsymbol{A}$ is an eigenoperator to the eigenvalue zero, then it is diagonal or at least nondiagonal only between degenerated states. Indeed from expanding the operator $\boldsymbol{A}$ in the basis of $\boldsymbol{L}_0$ and applying the eigenvalue equation follows

$$\boldsymbol{L}_0 \boldsymbol{A} = \boldsymbol{L}_0 \sum_\mu \sum_\nu A_{\mu\nu} |\mu\rangle\langle\nu| = \sum_\mu \sum_\nu A_{\mu\nu} (\varepsilon_\mu - \varepsilon_\nu) |\mu\rangle\langle\nu| = \boldsymbol{0} \tag{61}$$

Taking the matrix elements yields

$$0 \;=\; A_{\mu\nu}(\varepsilon_\mu - \varepsilon_\nu) \tag{62}$$

what proves the statement. Of course the same holds if $\boldsymbol{B}$ belongs to the eigenvalue zero. Furthermore, from eq (58) one can derive the following statement: If both operators $\boldsymbol{A}$ and $\boldsymbol{B}$ respectively are eigenoperators and at least one of them has the eigenvalue zero, then the expectation value vanishes or both eigenvalues are zero. Thus, for all nonvanishing expectation values both operators have to be diagonal, if one is. In the latter case the two operators commute. One can also prove the following statements, in some sense reverse to the above said. If two eigenoperators $\boldsymbol{A}$ and $\boldsymbol{B}$ anticommute their expectation value $\langle \boldsymbol{AB} \rangle$ vanishes. This follows from equation (59)

$$\langle \boldsymbol{AB} \rangle \;=\; \frac{1}{1 - e^{\beta\lambda_A}} \langle [\boldsymbol{A}, \boldsymbol{B}] \rangle \;=\; \frac{2}{1 - e^{\beta\lambda_A}} \langle \boldsymbol{AB} \rangle \tag{63}$$

but this means $\langle \boldsymbol{AB} \rangle = 0$. Furthermore, if two eigenoperators $\boldsymbol{A}$ and $\boldsymbol{B}$ commute their expectation value $\langle \boldsymbol{AB} \rangle$ either vanishes or both eigenvalues have to be zero. Indeed, we get from eq (55)

$$\langle \boldsymbol{AB} \rangle \;=\; \frac{1}{1 + e^{\beta\lambda_A}} \langle [\boldsymbol{A}, \boldsymbol{B}]_+ \rangle \;=\; \frac{2}{1 + e^{\beta\lambda_A}} \langle \boldsymbol{AB} \rangle \tag{64}$$

Again one possible solution is $\langle \boldsymbol{AB} \rangle = 0$, but if we demand that $\langle \boldsymbol{AB} \rangle \neq 0$ then necessarily $\lambda_A = 0$ holds. Besides λ_A also λ_B has to vanish which follows from eq (58). Thus the number of operators inside an expectation value can be reduced by help of eq (60) till all remaining operators are commuting and diagonal. For illustration, let us assume for the moment both $\boldsymbol{A}$ and $\boldsymbol{B}$ to be simple basis operators of the form

$$\boldsymbol{A} \;=\; |\mu\rangle\langle\mu'| \qquad \text{with} \qquad \lambda_A = \varepsilon_\mu - \varepsilon_{\mu'} \tag{65}$$

$$\boldsymbol{B} \;=\; |\nu\rangle\langle\nu'| \qquad \text{with} \qquad \lambda_B = \varepsilon_\nu - \varepsilon_{\nu'} \tag{66}$$

then we find

$$\langle [\boldsymbol{A}, \boldsymbol{B}]_+ \rangle \;=\; \left(e^{-\beta\varepsilon_\mu} + e^{-\beta\varepsilon_\nu} \right) \frac{\delta_{\mu\nu'}\delta_{\nu\mu'}}{Z_0} \tag{67}$$

$$\langle \boldsymbol{AB} \rangle \;=\; \frac{e^{-\beta\varepsilon_\mu} + e^{-\beta\varepsilon_\nu}}{e^{\beta(\varepsilon_\mu - \varepsilon_\nu)} + 1} \frac{\delta_{\mu\nu'}\delta_{\nu\mu'}}{Z_0} = \frac{e^{-\beta\varepsilon_\mu}}{Z_0} \delta_{\mu\nu'}\delta_{\nu\mu'} \tag{68}$$

For arbitrary non-diagonal operators

$$\boldsymbol{A} = \sum_{\mu\neq\nu} A_{\mu\nu} |\mu\rangle\langle\nu| \qquad \text{and} \qquad \boldsymbol{B} = \sum_{\mu'\neq\nu'} B_{\mu'\nu'} |\mu'\rangle\langle\nu'| \tag{69}$$

one finds

$$\langle \boldsymbol{AB} \rangle \;=\; \sum_{\mu\neq\nu} \frac{e^{-\beta\varepsilon_\mu}}{Z_0} A_{\mu\nu} B_{\nu\mu} \tag{70}$$

If we take both $\boldsymbol{A}$ and $\boldsymbol{B}$ to be the perturbation we get together with eq (97) the result for Z_2 in accordance with eq (36). In appendix C we show how eq (60) together with the statements given above can be utilized to evaluate expectation values within the Hubbard model in a systematic manner.

4 The one band Hubbard model

We will demonstrate it for the Hubbard model, being the most simple lattice fermion model taking into account electron electron interaction. In the context of strong electron correlation especially the perturbation expansion around the atomic limit is of interest. Therefore, we focus the discussion to that case. The Hamiltonian of the Hubbard model for a grand canonical ensemble is

$$\boldsymbol{H} \;=\; \boldsymbol{H}_0 + \boldsymbol{H}_1 \tag{71}$$

with

$$\boldsymbol{H}_0 \;=\; \sum_{i\sigma} \left(\frac{U}{2} \mathbf{n}_{i\sigma} \mathbf{n}_{i-\sigma} - (\mu + \sigma h_i) \mathbf{n}_{i\sigma} \right) \tag{72}$$

$$\boldsymbol{H}_1 \;=\; t \sum_{i \neq j\sigma} \mathbf{c}_{i\sigma}^+ \mathbf{c}_{j\sigma} \tag{73}$$

Here $\mathbf{c}_{i\sigma}^+$ and $\mathbf{c}_{i\sigma}$ are the creation and destruction operators in Wannier representation. The chemical potential μ and the magnetic field in z-direction are introduced to take the effects of doping and applying external magnetic fields into account. The model has two exact solveable limits, i.e. the band limit with $U = 0$ and the atomic limit, where $t = 0$ holds. Since we are interested in the large U limit, we use as unperturbed Hamiltonian $\boldsymbol{H}_0$, the so called atomic limit of the Hubbard model. Within this limit the electrons are at N independent lattice sites and the partition sum factorizes. The eigenoperators of the related Liouvillian $\boldsymbol{L}_0$ are the so called Hubbard operators [22] and products of them. Since the multisite Hilbertspace and also the related Liouville space are the direct product of the N single site spaces, it is enough to restrict the discussion to one lattice site indexed by i for the moment. For one lattice site the atomic limit Hamiltonian is

$$\boldsymbol{H}_i = U \mathbf{n}_{i\uparrow} \mathbf{n}_{i\downarrow} - h_i (\mathbf{n}_{i\uparrow} - \mathbf{n}_{i\downarrow}) - \mu (\mathbf{n}_{i\uparrow} + \mathbf{n}_{i\downarrow}) \tag{74}$$

and its Hilbertspace is spanned by the four eigenstates:

$\lvert i, 0 \rangle$	if the lattice site is empty,	(75)
$\lvert i, u \rangle$	if the lattice site is occupied with a spin-up electron,	(76)
$\lvert i, d \rangle$	if the lattice site is occupied with a spin-down electron,	(77)
$\lvert i, 2 \rangle$	if the lattice site is occupied with two electrons. .	(78)

The related eigenvalue equations are

$$\boldsymbol{H}_i \lvert i, \mu \rangle = \varepsilon_{i\mu} \lvert i, \mu \rangle \qquad \text{with} \qquad \mu, \nu \in \{0, u, d, 2\} \tag{79}$$

and

$$\varepsilon_{i0} = 0 \quad , \quad \varepsilon_{i\sigma} = -\sigma h_i - \mu \quad , \quad \varepsilon_{i2} = -2\mu + U \tag{80}$$

From these states one can construct the natural basis of the related operator space. This was also first done by Hubbard [22] indicating the basis operators by $X_i^{\mu\nu} = |i, \mu\rangle\langle i, \nu|$. The eigenvalue equation for the basis operators is

$$\boldsymbol{L}_i X_i^{\mu\nu} = \lambda_i^{\mu\nu} X_i^{\mu\nu} \qquad \text{with} \qquad \lambda_i^{\mu\nu} = \varepsilon_{i\mu} - \varepsilon_{i\nu} \quad . \tag{81}$$

For a detailed discussion of the physics of these operators and a related diagrammatic technique I refer to the book of Isjumov and Skrjabin [23] and the references therein. The fermion creation and destruction operators may be expressed via the basis operators according to

$$\mathbf{c}_{i\sigma} = X_i^{0\sigma} + \sigma X_i^{-\sigma 2} \tag{82}$$
$$\mathbf{c}_{i\sigma}^+ = X_i^{\sigma 0} + \sigma X_i^{2-\sigma} \tag{83}$$
$$\mathbf{n}_{i\sigma} = X_i^{\sigma\sigma} + X_i^{22} \tag{84}$$

and for the atomic limit Hamiltonian playing the role of $\boldsymbol{H}_0$ in the perturbation theory, we get

$$\boldsymbol{H}_0 = \sum_{i\sigma} \left((\frac{U}{2} - \mu)X_i^{22} - (\mu + \sigma h_i)X_i^{\sigma\sigma} \right) \tag{85}$$

The related partition sum is

$$Z_0 = \prod_i z_i \qquad \text{with} \qquad z_i = 1 + e^{\beta(\mu + h_i)} + e^{\beta(\mu - h_i)} + e^{\beta(2\mu - U)} \tag{86}$$

The partition sum factorizes into the product of N single site partition sums. By help of eqs (82,83) the hopping part may also be rewritten in terms of single site basis operators

$$\boldsymbol{H}_1 = t \sum_{i \neq j\sigma} \left(X_i^{\sigma 0} X_j^{0\sigma} + \sigma X_i^{\sigma 0} X_j^{-\sigma 2} + \sigma X_i^{2-\sigma} X_j^{0\sigma} + X_i^{2-\sigma} X_j^{-\sigma 2} \right) \tag{87}$$

Using the eigenvalue equation for the X-operators yields

$$\boldsymbol{L}_0 X_i^{\mu\nu} X_j^{\mu'\nu'} = (\lambda_i^{\mu\nu} + \lambda_j^{\mu',\nu'}) X_i^{\mu\nu} X_j^{\mu'\nu'} \tag{88}$$

Therefore, the operator $\boldsymbol{a}_{11}$ defined in eq (12) takes the following form

$$\boldsymbol{a}_{11} = -t \sum_r \sum_{i \neq j\sigma} \boldsymbol{A}_{ij\sigma}^r \tag{89}$$

Here I used the abbreviations

$$\boldsymbol{A}_{ij\sigma}^1 = X_i^{\sigma 0} X_j^{0\sigma} \tag{90}$$
$$\boldsymbol{A}_{ij\sigma}^2 = \sigma X_i^{\sigma 0} X_j^{-\sigma 2} \tag{91}$$
$$\boldsymbol{A}_{ij\sigma}^3 = \sigma X_i^{2-\sigma} X_j^{0\sigma} \tag{92}$$
$$\boldsymbol{A}_{ij\sigma}^4 = X_i^{2-\sigma} X_j^{-\sigma 2} \tag{93}$$

What remains, is to calculate the matrix elements of $\boldsymbol{a}_{11}$. The straight forward way is to define an eigenstate of $\boldsymbol{H}_0$ by help of the X-operators in the following way

$$|\{\mu\}\rangle \;=\; \prod_{l=1}^{N} X_l^{\mu_l 0}|\text{vac}\rangle \tag{94}$$

and to calculate the matrix elements. This lengthy calculation is interesting from a pedagogical point of view and we shift it to the appendix C. Here we adopt another way, starting from eq (30). Insertion of operator $\boldsymbol{a}_{11}$ in the form given in eq (89) yields for the Hubbard model

$$
\begin{aligned}
Z_2/Z_0 \;&=\; t^2 \sum_r \sum_{i\neq j\sigma} \sum_{r'} \sum_{k\neq l\sigma'} \left(\frac{\beta^2}{2!} + \sum_{n=3}^{\infty} \frac{\beta^n}{n!}(\lambda_{ij\sigma}^r)^{n-2} \right) \langle \boldsymbol{A}_{ij\sigma}^r \boldsymbol{A}_{kl\sigma'}^{r'} \rangle \\
&=\; t^2 \sum_r \sum_{i\neq j\sigma} \sum_{r'} \sum_{k\neq l\sigma'} f_2(\lambda_{ij\sigma}^r) \langle \boldsymbol{A}_{ij\sigma}^r \boldsymbol{A}_{kl\sigma'}^{r'} \rangle
\end{aligned} \tag{95}
$$

The third order term becomes with eq (31)

$$Z_3/Z_0 \;=\; -t^3 \sum_r \sum_{i\neq j\sigma} \sum_{r'} \sum_{i'\neq j'\sigma'} \sum_{r''} \sum_{i''\neq j''\sigma''} f_3(\lambda_{ij\sigma}^r, \lambda_{ij\sigma}^r + \lambda_{i'j'\sigma'}^{r'}) \langle \boldsymbol{A}_{ij\sigma}^r \boldsymbol{A}_{i'j'\sigma'}^{r'} \boldsymbol{A}_{i''j''\sigma''}^{r''} \rangle \tag{96}$$

Proceeding in the same way as before yields for contribution of order t^m

$$Z_m/Z_0 \;=\; (-t)^m \sum_{x_1} \cdots \sum_{x_m} f_m(\lambda_1, \ldots, \lambda_{m-1}) \langle \boldsymbol{A}_{x_1} \cdots \boldsymbol{A}_{x_m} \rangle \tag{97}$$

Here x_i abbreviates the set of indices r, i, j, and σ of the operator $\boldsymbol{A}_{ij\sigma}^r$. The meaning of λ_1, λ_2, and so on has a little bit changed with respect to eq (43), i.e.

$$
\begin{aligned}
\lambda_1 \;&=\; \lambda_{x_1} = \lambda_{ij\sigma}^r \\
\lambda_2 \;&=\; \lambda_{x_1} + \lambda_{x_2} \\
&\;\;\vdots \\
\lambda_k \;&=\; \sum_{i=1}^{k} \lambda_{x_i}
\end{aligned} \tag{98}
$$

The remaining task is to calculate the expectation values in eq (97). Since all the X-operators appearing in the perturbation are nondiagonal, all expectation values containing unpaired operators vanish. Thus we have to take into account all possible systems of paired X-operators, where a factor -1 has to be included, if the number of commutations necessary to make all pairing X operators neighbours is odd, a factor +1 otherwise. This is nothing but Wick's theorem. Of course most of these remaining expectation values vanish also, since not every X-operator fits to each other and the pairing of two operators may be on-site non-diagonal. Nevertheless after the first pairing step every expectation value containing 2m, what is two times the order in t, X-operators disintegrates into a finite series of expectation values containing m X-operators. In case that the lattice site indices of all remaining X-operators are different one from each other, we have to take

into account all terms containing diagonal X-operators. In case that some of the lattice site indices are equal we have to contract them again. This way one can systematically find all nonvanishing contributions to an m-order expectation value. The second order expectation value is

$$\langle \boldsymbol{A}^r_{ij\sigma} \boldsymbol{A}^{r'}_{mn\sigma'} \rangle = \langle X_i^{\alpha_i \alpha'_i} X_j^{\xi_j \xi'_j} X_m^{\gamma_m \gamma'_m} X_n^{\eta_n \eta'_n} \rangle \tag{99}$$

Due to the summation restriction $i \neq j$ and $m \neq n$ two contributions remain

$$\langle X_i^{\alpha_i \alpha'_i} X_j^{\xi_j \xi'_j} X_m^{\gamma_m \gamma'_m} X_n^{\eta_n \eta'_n} \rangle = \tag{100}$$
$$= -\langle X_i^{\alpha_i \gamma'_m} \rangle \delta_{im} \delta_{\alpha'_i \gamma_m} \langle X_j^{\xi_j \eta'_j} \rangle \delta_{jn} \delta_{\xi'_j \eta_n} + \langle X_i^{\alpha_i \eta'_n} \rangle \delta_{in} \delta_{\alpha'_i \eta_n} \langle X_j^{\xi_j \gamma'_m} \rangle \delta_{jm} \delta_{\xi'_j \gamma_m}$$
$$= \frac{e^{-\beta \varepsilon_{\alpha_i}}}{z_i} \frac{e^{-\beta \varepsilon_{\xi_j}}}{z_j} \left(-\delta_{im} \delta_{jn} \delta_{\alpha_i \gamma'_m} \delta_{\alpha'_i \gamma_m} \delta_{\xi_j \eta'_n} \delta_{\xi'_j \eta_n} + \delta_{in} \delta_{jm} \delta_{\alpha_i \eta'_n} \delta_{\alpha'_i \eta_n} \delta_{\xi_j \gamma'_m} \delta_{\xi'_j \gamma_m} \right)$$

Insertion into eq (95) shows, that only four out of the sixteen terms survive. What we get finally is

$$Z_2/Z_0 = t^2 \sum_{i \neq j} \sum_\sigma \left(\frac{e^{-\beta(\varepsilon_{i\sigma} + \varepsilon_{j0})}}{z_i z_j} f_2 \left(\varepsilon_{i\sigma} - \varepsilon_{i0} + \varepsilon_{j0} - \varepsilon_{j\sigma} \right) \right.$$
$$+ \frac{e^{-\beta(\varepsilon_{i\sigma} + \varepsilon_{j-\sigma})}}{z_i z_j} f_2 \left(\varepsilon_{i\sigma} - \varepsilon_{i0} + \varepsilon_{j-\sigma} - \varepsilon_{j2} \right)$$
$$+ \frac{e^{-\beta(\varepsilon_{i2} + \varepsilon_{j0})}}{z_i z_j} f_2 \left(\varepsilon_{i2} - \varepsilon_{i-\sigma} + \varepsilon_{j0} - \varepsilon_{j\sigma} \right)$$
$$\left. + \frac{e^{-\beta(\varepsilon_{i2} + \varepsilon_{j-\sigma})}}{z_i z_j} f_2 \left(\varepsilon_{i2} - \varepsilon_{i-\sigma} + \varepsilon_{j-\sigma} - \varepsilon_{j2} \right) \right) \tag{101}$$

With eqs (80) we get therefore

$$Z_2/Z_0 = t^2 \sum_{i \neq j} \sum_\sigma \left(\frac{e^{\beta(\mu + \sigma h_i)}}{z_i z_j} f_2 \left(-\sigma(h_i - h_j) \right) + \frac{e^{\beta(2\mu + \sigma(h_i - h_j))}}{z_i z_j} f_2 \left(-\sigma(h_i - h_j) - U \right) \right.$$
$$\left. + \frac{e^{\beta(2\mu - U)}}{z_i z_j} f_2 \left(U - \sigma(h_i - h_j) \right) + \frac{e^{\beta(3\mu - U - \sigma h_j)}}{z_i z_j} f_2 \left(-\sigma(h_i - h_j) \right) \right) \tag{102}$$

Although the above formula holds for arbitrary magnetic fields, we restrict here to the most discussed ferromagnetic and antiferromagnetic cases and admit nearest neighbour hopping only. For a homogenous magnetic field, i.e. $h_i = h_j = h$, we find

$$Z_2 = Z_0 N g t^2 \sum_\sigma \left(\frac{e^{\beta(\mu + \sigma h)}}{z^2(h)} f_2(0) + \frac{e^{\beta 2\mu}}{z^2(h)} f_2(-U) \right.$$
$$\left. + \frac{e^{\beta(2\mu - U)}}{z^2(h)} f_2(U) + \frac{e^{\beta(3\mu - U - \sigma h)}}{z^2(h)} f_2(0) \right) \tag{103}$$

Here N is the number of lattice sites and g the number of nearest neighbours. For a staggered magnetic field, i.e. $h_i = -h_j$ with $h_i = h_s$ on the A sublattice and $h_i = -h_s$ on the B sublattice, we have

$$Z_2 = Z_0 N g t^2 \sum_\lambda \left(\frac{e^{\beta(\mu + \lambda h_s)}}{z^2(h_s)} f_2(-2\lambda h_s) + \frac{e^{\beta(2\mu + 2\lambda h_s)}}{z^2(h_s)} f_2(-2\lambda h_s - U) \right.$$
$$\left. + \frac{e^{\beta(2\mu - U)}}{z^2(h_s)} f_2(U - 2\lambda h_s) + \frac{e^{\beta(3\mu - U - \lambda h_s)}}{z^2(h_s)} f_2(-2\lambda h_s) \right) \quad (104)$$

with

$$\lambda = \begin{cases} 1 & \text{for } i \in A \text{ and } \sigma = +1 \quad \text{or for } i \in B \text{ and } \sigma = -1 \\ -1 & \text{for } i \in A \text{ and } \sigma = -1 \quad \text{or for } i \in B \text{ and } \sigma = +1 \end{cases} \quad (105)$$

We compared our second order result given in eq (102) to that given in [13, 15, 18, 19] and found it in complete accordance. Here we restrict ourself to the second order since we believe it is enough to demonstrate the reliability of the presented perturbation theory. The calculation of higher order terms and discussion of the physics contained therein we shift to a forthcoming paper.

5   Conclusion

The main result of this paper is condensed in eq (44), since it contains the time integrations. We showed here the derivation via recursive relations, since this way it is palpably that the degenerate case is included and does not generate any problems. Furthermore, the recursive relation for the operators a_{nm} can be solved easily in symbolic manner by help of symbolic computer algebra programs. Once knowing the factor f_m, the remaining task, i.e. the calculation of the diagonal matrix elements, is straight forward. Since linked graphs have to be evaluated only, the further calculation steps are very likely to the coupled cluster expansion. In [19] the authors did the time integrals by symbolic computation. In our theory this step is economized. At the first glance one might think that this benefit is paid by the disadvantage that one cannot permute the indices due to the weigth factors $f_m(\lambda_1, \ldots, \lambda_{m-1})$. This is not the case due to the inherent symmetries of the functions f_m. Furthermore, since these functions remain finite for arbitrary sets of energies, the case of degeneration is included what is important for the typical models of strong electron correlation. Nevertheless, it remains cumbersome enough to calculate all the linked diagrams in higher orders. The reduction via commutations as shown in the appendix C is suited for symbolic computer algebra. In case of the Hubbard model the result for every cluster is a sum of products of Kronecker symbols and single-site expectation values of the X-operators, selecting a set of energy eigenvalues which specify the values of the $\lambda's$ in the functions f_m. The form of the theory given in section 2 seems to exhibit slight differences compared to the variant given in section 4 for the Hubbard model. This stems from the fact, that in section 2 the perturbation was treated without

knowledge of its inner structure, whereas in section 4 we made use of this knowledge. If the special form is known, one can calculate $V_{\mu\nu}$ as was demonstrated in appendix B, thus showing both variants to be identical.

Appendices

Appendix A: Green function technique for eigenoperators

We define the retarded Greens function with respect to the operator $\boldsymbol{H}_0$ in the usual way [11]

$$\langle\langle \boldsymbol{A}(t)\,;\,\boldsymbol{B}\rangle\rangle \;\;=\;\; -i\Theta(t)\langle[\boldsymbol{A}(t),\boldsymbol{B}]_+\rangle \tag{106}$$

$\Theta(t)$ is the step function, and

$$\boldsymbol{A}(t) \;\;=\;\; e^{it\boldsymbol{H}_0}\boldsymbol{A}e^{-it\boldsymbol{H}_0} = e^{it\boldsymbol{L}_0}\boldsymbol{A} \tag{107}$$

The Fourier-transformed equation of motion is than

$$\omega\langle\langle \boldsymbol{A}\,;\,\boldsymbol{B}\rangle\rangle_\omega \;\;=\;\; \langle[\boldsymbol{A},\boldsymbol{B}]_+\rangle - \langle\langle \boldsymbol{L}_0\boldsymbol{A}\,;\,\boldsymbol{B}\rangle\rangle_\omega \tag{108}$$

Due to the eigenvalue equation holding for the eigenoperator $\boldsymbol{A}$ this can be solved for the wanted Greens function

$$\langle\langle \boldsymbol{A}\,;\,\boldsymbol{B}\rangle\rangle_\omega \;\;=\;\; \frac{\langle[\boldsymbol{A},\boldsymbol{B}]_+\rangle}{\omega + \lambda_A} \tag{109}$$

The expectation values $\langle\boldsymbol{B}\boldsymbol{A}\rangle$ one gets via the spectral theorem

$$\begin{aligned}
\langle\boldsymbol{B}\boldsymbol{A}\rangle \;\;&=\;\; \lim_{\delta\to\infty}\frac{i}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega}{e^{\beta\omega}+1}\left\{\langle\langle \boldsymbol{A}\,;\,\boldsymbol{B}\rangle\rangle_{\omega+i\delta} - \langle\langle \boldsymbol{A}\,;\,\boldsymbol{B}\rangle\rangle_{\omega-i\delta}\right\} \\
&=\;\; \frac{\langle[\boldsymbol{A},\boldsymbol{B}]_+\rangle}{e^{-\beta\lambda_A}+1}
\end{aligned} \tag{110}$$

This is the same result as given in eq (55).

Appendix B: The straight way

First we calculate the matrix elements of $\boldsymbol{a}_{11}$. To this end we define an eigenstate of $\boldsymbol{H}_0$ by help of the X operators in the following way

$$|\{\mu\}\rangle \;\;=\;\; \prod_{l=1}^{N} X_l^{\mu_l 0}|\text{vac}\rangle \tag{111}$$

Here $\{\mu\}$ stands for a set $\{\mu_1, ..., \mu_N\}$, summation over $\{\mu\}$ means N sums over the μ_i. The matrix elements to calculate are of the form

$$\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}X_j^{\xi_j\xi_j'}|\{\nu\}\rangle \tag{112}$$

Insertion of a unit operator yields

$$\sum_{\{\gamma\}}\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}|\{\gamma\}\rangle\langle\{\gamma\}|X_j^{\xi_j\xi_j'}|\{\nu\}\rangle \tag{113}$$

For the matrix element of a X-operator we find

$$\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}|\{\nu\}\rangle =$$
$$\langle\mathrm{vac}|\left(\prod_{l=1}^{i-1}X_l^{0\mu_l}\right)X_i^{0\nu_i}\left(\prod_{l=i+1}^{N}X_l^{0\mu_l}\right)X_i^{\alpha_i\alpha_i'}\left(\prod_{l'=N}^{i+1}X_{l'}^{\nu_{l'}}\right)X_i^{\nu_i0}\left(\prod_{l=i-1}^{1}X_{l'}^{\nu_{l'}}\right)|\mathrm{vac}\rangle \tag{114}$$

Now commuting the X_i operators to the center yields

$$\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}|\{\nu\}\rangle =$$
$$(-1)^{P(\{\mu\}_{i+1}^N|0\mu_i)}(-1)^{P(\nu_i0|\{\nu\}_N^{i+1})}\langle\mathrm{vac}|\left(\prod_{l\neq i}X_l^{0\mu_l}\right)X_i^{0\mu_i}X_i^{\alpha_i\alpha_i'}X_i^{\nu_i0}\left(\prod_{l'\neq i}X_{l'}^{\nu_{l'}0}\right)|\mathrm{vac}\rangle \tag{115}$$

Here we used the parity function introduced in eq (60). The three X-operators at lattice site i implode according to

$$X_i^{0\mu_i}X_i^{\alpha_i\alpha_i'}X_i^{\nu_i0} = X_i^{00}\delta_{\mu_i\alpha_i}\delta_{\alpha_i'\nu_i} \tag{116}$$

Since X_i^{00} is bosonic, moving it to the upmost right (or left) will not change the sign. Furthermore it does not alter the vacuum, so that it may be omitted. What results is

$$\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}|\{\nu\}\rangle =$$
$$(-1)^{P(\{\mu\}_{i+1}^N|0\mu_i)}(-1)^{P(\nu_i0|\{\nu\}_N^{i+1})}\delta_{\mu_i\alpha_i}\delta_{\alpha_i'\nu_i}\langle\mathrm{vac}|\left(\prod_{l\neq i}X_l^{0\mu_l}\right)\left(\prod_{l'\neq i}X_{l'}^{\nu_{l'}0}\right)|\mathrm{vac}\rangle \tag{117}$$

Due to the orthogonality of the eigenfunctions we find finally

$$\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}|\{\nu\}\rangle = (-1)^{P(\{\mu\}_{i+1}^N|0\mu_i)}(-1)^{P(\nu_i0|\{\nu\}_N^{i+1})}\delta_{\mu_i\alpha_i}\delta_{\alpha_i'\nu_i}\prod_{l\neq i}\delta_{\mu_l,\nu_l} \tag{118}$$

Another way to simplify the same matrix element is to change $X_i^{\alpha_i\alpha_i'}$ either to the left till it is the right neighbour of $X_i^{0\mu_i}$ yielding

$$\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}|\{\nu\}\rangle = (-1)^{P(\{\mu\}_{i+1}^N|\alpha_i\alpha_i')}\delta_{\mu_i\alpha_i}\delta_{\alpha_i'\nu_i}\prod_{l\neq i}\delta_{\mu_l,\nu_l} \tag{119}$$

or to the right till it is the left neighbour of $X_i^{\nu_i 0}$ resulting in

$$\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}|\{\nu\}\rangle = (-1)^{P(\alpha_i\alpha_i'|\{\nu\}_N^{i+1})}\delta_{\mu_i\alpha_i}\delta_{\alpha_i'\nu_i}\prod_{l\neq i}\delta_{\mu_l,\nu_l} \tag{120}$$

The different forms can be created also by applying the following rules holding for the parity function $P(\boldsymbol{A}|\boldsymbol{B})$

$$P(\boldsymbol{A}|\boldsymbol{B}) = P(\boldsymbol{B}|\boldsymbol{A}) \tag{121}$$
$$P(\boldsymbol{A}|\boldsymbol{BC}) = P(\boldsymbol{A}|\boldsymbol{CB}) \tag{122}$$
$$P(\boldsymbol{A}|\boldsymbol{BC}) = P(\boldsymbol{A}|\boldsymbol{B}) + P(\boldsymbol{A}|\boldsymbol{C}) \tag{123}$$
$$P(\boldsymbol{A}|\boldsymbol{BC}) = P(\boldsymbol{A}|\boldsymbol{BDDC}) = P(\boldsymbol{A}|\boldsymbol{BD}) + P(\boldsymbol{A}|\boldsymbol{DC}) \tag{124}$$

Thus we get for the matrix element in eq (112)

$$\langle\{\mu\}|X_i^{\alpha_i\alpha_i'}X_j^{\xi_j\xi_j'}|\{\nu\}\rangle$$
$$= \sum_{\{\gamma\}}(-1)^{P(\alpha_i\alpha_i'|\{\mu\}_{i+1}^N)}\delta_{\mu_i\alpha_i}\delta_{\alpha_i'\gamma_i}\prod_{l\neq i}\delta_{\mu_l,\gamma_l}(-1)^{P(\xi_j\xi_j'|\{\nu\}_N^{j+1})}\delta_{\gamma_j\xi_j}\delta_{\xi_j'\nu_j}\prod_{l'\neq j}\delta_{\gamma_{l'},\nu_{l'}}$$
$$= (-1)^{P(\alpha_i\alpha_i'|\{\mu\}_{i+1}^N)}(-1)^{P(\xi_j\xi_j'|\{\nu\}_N^{j+1})}\delta_{\mu_i\alpha_i}\delta_{\alpha_i'\nu_i}\delta_{\mu_j\xi_j}\delta_{\xi_j'\nu_j}\prod_{l\neq i,j}\delta_{\mu_l,\nu_l} \tag{125}$$

with this result we find the matrix elements of the perturbation to be

$$\langle\{\mu\}|\boldsymbol{H}_1|\{\nu\}\rangle = -t\prod_{l\neq i,j}\delta_{\mu_l\nu_l}\sum_{i\neq j}\sum_{\sigma}(-1)^{P(f|\{\mu\}_{i+1}^N)}(-1)^{P(f|\{\nu\}_N^{j+1})}\times$$
$$\times(\delta_{\mu_i\sigma}\delta_{0\nu_i}+\sigma\delta_{\mu_i 2}\delta_{-\sigma\nu_i})(\delta_{\mu_j 0}\delta_{\sigma\nu_j}+\sigma\delta_{\mu_j-\sigma}\delta_{2\nu_i}) \tag{126}$$

Here we used the fact that both $X_i^{\sigma 0}$ and $X_i^{2-\sigma}$ are fermionic and we abbreviated both with f. The second order contribution to the partition sum reads now

$$Z_2 = t^2\sum_{i\neq j}\sum_{\sigma}\sum_{m\neq n}\sum_{\sigma'}\sum_{\{\mu\}}\sum_{\{\nu\}}e^{-\beta E_{\{\mu\}}}f_2(E_{\{\mu\}}-E_{\{\nu\}})\prod_{l\neq i,j}\delta_{\mu_l\nu_l}\prod_{l'\neq i,j}\delta_{\mu_{l'}\nu_{l'}}\times \tag{127}$$
$$\times(-1)^{P(f|\{\mu\}_{i+1}^N)}(-1)^{P(f|\{\nu\}_N^{j+1})}(-1)^{P(f|\{\nu\}_{m+1}^N)}(-1)^{P(f|\{\mu\}_N^{n+1})}$$
$$\times(\delta_{\mu_i\sigma}\delta_{0\nu_i}+\sigma\delta_{\mu_i 2}\delta_{-\sigma\nu_i})(\delta_{\mu_j 0}\delta_{\sigma\nu_j}+\sigma\delta_{\mu_j-\sigma}\delta_{2\nu_i})$$
$$\times(\delta_{\nu_m\sigma'}\delta_{0\mu_m}+\sigma'\delta_{\nu_m 2}\delta_{-\sigma'\mu_m})(\delta_{\nu_n 0}\delta_{\sigma'\mu_n}+\sigma'\delta_{\nu_n-\sigma'}\delta_{2\mu_n'})$$

Next we carry out the $\{\nu\}$-sum. All contributions where the indices i,j are distinct from m and n vanishes due to the fact that the X-operators within the perturbation are non-diagonal. What remains are the two contributions according to i=m, j=n and i=n, j=m. The first contribution also vanishes, what may be shown by doing the same steps we shall employ in the following for the calculation of the nonvanishing second case. Introducing the shortcut $\{\mu\}_{/ij}$ for the set of μ's except μ_i and μ_j we find

$$Z_2 = t^2\sum_{i\neq j}\sum_{\sigma}\sum_{\{\mu\}_{/ij}}e^{-\beta E(\{\mu\}_{/ij})}\sum_{\mu_i\mu_j}\sum_{\nu_i\nu_j}e^{-\beta(\varepsilon_{\mu_i}+\varepsilon_{\mu_j})}f_2(\varepsilon_{\mu_i}+\varepsilon_{\mu_j}-\varepsilon_{\nu_i}+\varepsilon_{\nu_j})\times$$

$$\times (-1)^{P(f|\{\mu\}_{i+1}^N)}(-1)^{P(f|\{\mu\}_N^{i+1})}$$

$$\times \left(\delta_{j>i}(-1)^{P(f|\{\mu\}_N^{j+1})}(-1)^{P(f|\{\mu\}_{j+1}^N)} + \delta_{j<i}(-1)^{P(f|\{\mu\}_N^{i+1}\nu_i\{\mu\}_{i-1}^{j+1})}(-1)^{P(f|\{\mu\}_N^{i+1}\nu_i\{\mu\}_{i-1}^{j+1})} \right)$$

$$\times (\delta_{\mu_i\sigma}\delta_{0\nu_i} + \sigma\delta_{\mu_i 2}\delta_{-\sigma\nu_i})(\delta_{\mu_j 0}\delta_{\sigma\nu_j} + \sigma\delta_{\mu_j - \sigma}\delta_{2\nu_i})$$

$$\times (\delta_{\nu_j\sigma'}\delta_{0\mu_j} + \sigma'\delta_{\nu_j 2}\delta_{-\sigma'\mu_j})(\delta_{\nu_i 0}\delta_{\sigma'\mu_i} + \sigma'\delta_{\nu_i - \sigma'}\delta_{2\mu_i'})$$

By help of the rules given for the parity function eqs (121,122,123,124) it is easy to show that we get a plus sign. Expanding the products, we find that only four out of the sixteen terms survive

$$Z_2 = t^2 \sum_{i \neq j} \sum_\sigma \sum_{\{\mu\}_{/ij}} e^{-\beta E(\{\mu\}_{/ij})} \sum_{\mu_i \mu_j} \sum_{\nu_i \nu_j} e^{-\beta(\varepsilon_{\mu_i} + \varepsilon_{\mu_j})} f_2(\varepsilon_{\mu_i} + \varepsilon_{\mu_j} - \varepsilon_{\nu_i} + \varepsilon_{\nu_j}) \times$$

$$\times (\delta_{\mu_i\sigma}\delta_{0\nu_i}\delta_{\sigma\sigma'} + \sigma\sigma'\delta_{\mu_i 2}\delta_{-\sigma\nu_i}\delta_{\sigma\sigma'})(\delta_{\mu_j 0}\delta_{\sigma\nu_j}\delta_{\sigma\sigma'} + \sigma\delta_{\mu_j - \sigma}\delta_{2\nu_i}) + \sigma\sigma'\delta_{\mu_j 2}\delta_{-\sigma\nu_j}\delta_{\sigma\sigma'} \quad (128)$$

Summing over $\mu_i, \mu_j, \nu_i, \nu_j$ and σ' yields

$$Z_2 = t^2 \sum_{\{\mu\}_{/ij}} e^{-\beta E(\{\mu\}_{/ij})} \sum_{i \neq j} \sum_\sigma \times$$

$$\times \left\{ e^{-\beta(\varepsilon_{i\sigma} + \varepsilon_{j0})} f_2(\varepsilon_{i\sigma} + \varepsilon_{j0} - \varepsilon_{i0} - \varepsilon_{j\sigma}) \right.$$

$$+ e^{-\beta(\varepsilon_{i\sigma} + \varepsilon_{j-\sigma})} f_2(\varepsilon_{i\sigma} + \varepsilon_{j-\sigma} - \varepsilon_{i0} - \varepsilon_{j2})$$

$$+ e^{-\beta(\varepsilon_{i2} + \varepsilon_{j0})} f_2(\varepsilon_{i2} + \varepsilon_{j0} - \varepsilon_{i-\sigma} - \varepsilon_{j\sigma})$$

$$\left. + e^{-\beta(\varepsilon_{i2} + \varepsilon_{j-\sigma})} f_2(\varepsilon_{i2} + \varepsilon_{j-\sigma} - \varepsilon_{i-\sigma} - \varepsilon_{j2}) \right\} \quad (129)$$

The sum over $\{\mu\}_{/ij}$ may be expressed by the unperturbed partition sum according to

$$\sum_{\{\mu\}_{/ij}} e^{-\beta E(\{\mu\}_{/ij})} = \frac{Z_0}{z_i z_j} \quad (130)$$

with z_i beeing the unperturbed single site partition sum. Thus we get exactly the same result of the second order contribution to the partition sum as was given in eq (102). The reader might have got the impression, that the method is complicated due to the multitude of factors $(-1)^P(\{\cdots\}|\{\cdots\})$ containing dummy lattice sites. This is a result of our aim to demonstrate here the straight forward character of the theory instead of modifying it to the special case of the Hubbard model. The straight calculation consists of firstly writing down the expression of Z_m in dependence of the $\lambda_1, \cdots, \lambda_{m-1}$, secondly one has to calculate the matrix elements of the perturbation with respect to the unperturbed (many body) states, and thirdly one has to multiply the mth power of that matrix to the known function $f_m(\lambda_1, \cdots, \lambda_{m-1})$. This way we have not to evaluate any graphs or difficult Green functions, instead simple matrix multiplications have to be carried out, thereby specifying the λ's, what is very comfortable as long as the dimension of the matrix is not to large, what is the case for instance in small cluster problems. In condensed matter systems, especially if one is interested in the limit $N \to \infty$, other methods can be utilized, as was shown for the Hubbard model in section 4.

Appendix C: Systematic evaluation via commutations

For an automated calculation Wick's theorem for the X-operators is not very convenient. A more systematic calculation starts from eq (60). Again it should be demonstrated for the evaluation of the second order expectation values, having the form given in eq (99). In the first step all X-operators are fermionic and we get therefore

$$
\begin{aligned}
\langle X_i^{\alpha\alpha'} X_j^{\xi\xi'} X_m^{\gamma\gamma'} X_n^{\eta\eta'} \rangle &= \frac{1}{e^{\beta\lambda_i^{\alpha\alpha'}} + 1} \langle [X_i^{\alpha\alpha'}, X_j^{\xi\xi'} X_m^{\gamma\gamma'} X_n^{\eta\eta'}]_+ \rangle \\
&= \frac{-\delta_{im}}{e^{\beta\lambda_i^{\alpha\alpha'}} + 1} \left(\delta_{\alpha'\gamma} \langle X_j^{\xi\xi'} X_i^{\alpha\gamma'} X_n^{\eta\eta'} \rangle + \delta_{\alpha\gamma'} \langle X_j^{\xi\xi'} X_i^{\gamma\alpha'} X_n^{\eta\eta'} \rangle \right) \\
&\quad + \frac{\delta_{in}}{e^{\beta\lambda_i^{\alpha\alpha'}} + 1} \left(\delta_{\alpha'\eta} \langle X_j^{\xi\xi'} X_m^{\gamma\gamma'} X_i^{\alpha\eta'} \rangle + \delta_{\alpha\eta'} \langle X_j^{\xi\xi'} X_m^{\gamma\gamma'} X_i^{\eta\alpha'} \rangle \right) \quad (131)
\end{aligned}
$$

Here we used the fact $i \neq j$. In the next step we have to calculate the product of three X-operators. Since in the general form used here, it is possible that e.g. $X_i^{\alpha\gamma'}$ is either fermionic or bosonic, we have to take into account the parity function. As an example we show here the calculation of only one of these expectation values

$$
\begin{aligned}
\langle X_j^{\xi\xi'} X_i^{\alpha\gamma'} X_n^{\eta\eta'} \rangle &= \frac{1}{1 - ge^{\beta\lambda_j^{\xi\xi'}}} \langle [X_j^{\xi\xi'}, X_i^{\alpha\gamma'} X_n^{\eta\eta'}]_g \rangle \\
&= \frac{(-1)^{P(X_j^{\xi\xi'}|X_i^{\alpha\gamma'})}\delta_{jn}}{1 - ge^{\beta\lambda_j^{\xi\xi'}}} \left(\delta_{\xi'\eta} \langle X_i^{\alpha\gamma'} X_j^{\xi\eta'} \rangle + \delta_{\xi\eta'} \langle X_i^{\gamma\alpha'} X_j^{\eta\xi'} \rangle \right) \quad (132) \\
g &= (-1)^{P(X_j^{\xi\xi'}|X_i^{\alpha\gamma'} X_n^{\eta\eta'})}
\end{aligned}
$$

Since we have $i \neq j$ the operators $X_i^{\gamma\alpha'}$ and $X_j^{\eta\xi'}$ either commute or anticommute. It follows from the statements given in section 3 that the expectation value of two (anti-)commuting X-operators at different lattice sites $\langle X_i^{\alpha\alpha'} X_j^{\xi\xi'} \rangle$ is zero except that $\lambda_i^{\alpha\alpha'} = 0$ and $\lambda_j^{\xi\xi'} = 0$ hold simultaneously, what means here that we have $\varepsilon_\alpha = \varepsilon_{\alpha'}$ and $\varepsilon_\xi = \varepsilon_{\xi'}$ or equivalently $\alpha = \alpha'$ and $\xi = \xi'$. In a condensed form this reads

$$
\langle X_i^{\alpha\alpha'} X_j^{\xi\xi'} \rangle = \langle X_i^{\alpha\alpha} X_j^{\xi\xi} \rangle \delta_{\alpha\alpha'} \delta_{\xi\xi'} \quad (133)
$$

For the remaining expectation value $\langle X_i^{\alpha\alpha} X_j^{\xi\xi} \rangle$ one finds by a direct calculation using eq (125) $X_i^{\alpha\alpha}$ and $X_j^{\xi\xi}$

$$
\langle X_i^{\alpha\alpha} X_j^{\xi\xi} \rangle = \frac{e^{-\beta\varepsilon_{i\alpha}}}{z_i} \frac{e^{-\beta\varepsilon_{j\xi}}}{z_j} \quad (134)
$$

Appendix D: An alternate derivation of f_m

This alternate derivation was given by Walter John after critical reading the manuscript of this paper.

In the following we start from

$$f_m(\beta; \lambda_1, \ldots, \lambda_{m-1}) = \int_0^\beta d\beta_1 \int_0^{\beta_1} d\beta_2 \cdots \int_0^{\beta_{m-1}} d\beta_m e^{\beta_1 \lambda_1} e^{\beta_2(-\lambda_1 + \lambda_2)} \ldots e^{\beta_m(-\lambda_{m-1})} \quad (135)$$

Here we mentioned the parameter β explicitly. The Laplace transformed function is then

$$F_m(p; \lambda_1, \ldots, \lambda_{m-1}) = \int_0^\infty d\beta e^{-p\beta} f_m(\beta; \lambda_1, \ldots, \lambda_{m-1}) \quad (136)$$

Partial integration yields

$$F_m(p; \lambda_1, \ldots, \lambda_{m-1}) = \left[\frac{e^{-p\beta}}{-p} f_m(\beta; \lambda_1, \ldots, \lambda_{m-1}) \right]_0^\infty \quad (137)$$

$$+ \frac{1}{p} \int_0^\infty d\beta e^{-(p - \lambda_1)\beta} \int_0^\beta d\beta_2 e^{\beta_2(-\lambda_1 + \lambda_2)} \int_0^{\beta_2} d\beta_3 \cdots \int_0^{\beta_{m-1}} d\beta_m e^{\beta_m(-\lambda_{m-1})}$$

The first term on the right hand side vanishes, if p is chosen adequately. Integrating by parts another time delivers

$$F_m(p; \lambda_1, \ldots, \lambda_{m-1}) = \quad (138)$$

$$\frac{1}{p} \frac{1}{p - \lambda_1} \int_0^\infty d\beta e^{-(p - \lambda_2)\beta} \int_0^\beta d\beta_3 e^{\beta_3(-\lambda_2 + \lambda_3)} \int_0^{\beta_3} d\beta_4 \cdots \int_0^{\beta_{m-1}} d\beta_m e^{\beta_m(-\lambda_{m-1})}$$

Thus from repeated partial integrations one gets finally

$$F_m(p; \lambda_1, \ldots, \lambda_{m-1}) = \frac{1}{p^2} \prod_{i=1}^{m-1} \frac{1}{p - \lambda_i} \quad (139)$$

The original function one gets via back-transforming

$$f_m(\beta; \lambda_1, \ldots, \lambda_{m-1}) = \frac{1}{2\pi i} \int_{C - i\infty}^{C + i\infty} dp \, e^{p\beta} F_m(p; \lambda_1, \ldots, \lambda_{m-1}) \quad (140)$$

Here C is a real constant larger than the maximum λ_i. The integration path may be deformed to encircle the individual poles lying on the real axes. Thus we get from Cauchy's theorem

$$f_m(\beta; \lambda_1, \ldots, \lambda_{m-1}) = \sum_{i=1}^{m-1} \frac{e^{\beta \lambda_i}}{\lambda_i^2} \frac{1}{\prod_{j \neq i}^{m-1}(\lambda_i - \lambda_j)} + \frac{1}{\prod_{j=1}^{m-1}(-\lambda_j)} \left(\beta + \sum_{i=1}^{m-1} \frac{1}{\lambda_i} \right) \quad (141)$$

The second term on the right hand side stems from the double pole at zero. Here we admitted only simple poles to get a concise form. There is no problem with the degenerate case, since in case that a pole has a higher order, one has to take higher derivatives during application of Cauchy's theorem. Via substitution of the exponential factor by help of eq (40) one can show the derived formula to be equivalent to eq (44).

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